FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
	FILING DATE February 18, 2000	GROUP 1631

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AM	AA1	4,811,217	03/1989	Tokizane *et al.*	364	300	
AM	AB1	4,859,736	08/1989	Rink	525	54.1	
AM	AC1	4,908,773	03/1990	Pantoliano *et al.*	364	496	
AM	AD1	4,935,875	06/1990	Shah *et al.*	364	497	
AM	AE1	4,939,666	07/1990	Hardman	364	496	
AM	AF1	5,010,175	04/1991	Rutter *et al.*	530	334	
AM	AG1	5,025,388	06/1991	Cramer, III *et al.*	364	496	
AM	AH1	5,155,801	10/1992	Lincoln	395	22	
AM	AI1	5,167,009	11/1992	Skeirik	395	27	
AM	AJ1	5,240,680	08/1993	Zuckerman *et al.*	422	67	
AM	AK1	5,260,882	11/1993	Blanco *et al.*	364	499	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AM	AL1	0 355 266 B1	06/1993	EP, Hudson et al.	B01J	19/00	Yes No
AM	AM1	0 355 628 B1	11/1993	EP, Gasson et al.	G21F	9/00	Yes No
AM	AN1	0 770 876 A1	05/1997	EP, Pakula et al.	G01N	33/68	Yes No
AM	AO1	0 818 744 A2	01/1998	EP, Young et al.	G06F	17/50	Yes No
AM	AP1	WO 91/19735	12/1991	PCT, Bartlett et al.	C07K	7/02	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	1	"3DP Gains drug research patent," Source of publication unclear, Vol. 32, No. 1, January 1996, 2 pages.
	~~AS~~	~~1~~	~~"Accelerate the Discovery Cycle with Chem-X!," Source and date of publication unclear, 2 pages.~~
AM	AT	1	Agrafiotis, D.k., "A New Method for Analyzing Protein Sequence Relationships Based on Sammon Maps," *Protein Science*, Vol. 6, No. 2, February 1997, pp. 287-293.

EXAMINER	Andrew Marschel	DATE CONSIDERED	9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AM	AA2	5,265,030	11/1993	Skolnick *et al.*	364	496	
AM	AB2	5,270,170	12/1993	Schatz *et al.*	435	7.37	
AM	AC2	5,288,514	02/1994	Ellman	427	2	
AM	AD2	5,307,287	04/1994	Cramer, III *et al.*	364	496	
AM	AE2	5,331,573	07/1994	Balaji *et al.*	364	500	
AM	AF2	5,434,796	07/1995	Weininger	364	496	
AM	AG2	5,436,850	07/1995	Eisenberg *et al.*	364	496	
AM	AH2	5,442,122	08/1995	Noda *et al.*	564	426	
AM	AI2	5,463,564	10/1995	Agrafiotis *et al.*	364	496	
AM	AJ2	5,499,193	03/1996	Sugawara *et al.*	364	500	
AM	AK2	5,519,635	05/1996	Miyake *et al.*	364	497	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AM	AL2	WO 92/00091	01/1992	PCT, Lam et al.	A61K	37/02	Yes No
AM	AM2	WO 93/20242	10/1993	PCT, Lerner et al.	C12Q	1/70	Yes No
AM	AN2	WO 94/28504	12/1994	PCT, Ragnan et al.	G06F	15/60	Yes No
AM	AO2	WO 95/01606	01/1995	PCT, Weininger	G06F	15/42	Yes No
AM	AP2	WO 97/09342	03/1997	PCT, Arenas et al.	C07H	21/02	Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	2	Agrafiotis, D.K., *et al.*, "Stochastic Algorithms for Maximizing Molecular Diversity," *Journal of Chemical Information and Computer Sciences*, Vol. 37, pp. 841-851, (1997).
AM	AS	2	Alsberg, B.K. *et al.*, "Classification of pyrolysis mass spectra by fuzzy multivariate rule induction-comparison with regression, K-nearest neighbor, neural and decision-tree methods," *Analytica Chimica Acta*, Vol. 348, No. 1-3, pp. 389-407, (August 20, 1997).
AM	AT	2	Amzel, L.M., "Structure-based drug design," *Current Opinion in Biotechnology*, Vol. 9, No. 4, August 1998, pp. 366-369.

EXAMINER	Sudha Mascarenhas	DATE CONSIDERED	9/23/02

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AM	AA3	5,526,281	06/1996	Chapman *et al.*	364	496	
AM	AB3	5,545,568	08/1996	Ellman	436	518	
AM	AC3	5,549,974	08/1996	Holmes	428	403	
AM	AD3	5,565,325	10/1996	Blake	435	7.1	
AM	AE3	5,574,656	11/1996	Agrafiotis *et al.*	364	500	
AM	AF3	5,585,277	12/1996	Bowie *et al.*	436	518	
AM	AG3	5,602,755	02/1997	Ashe *et al.*	364	498	
AM	AH3	5,612,895	03/1997	Balaji *et al.*	364	496	
AM	AI3	5,634,017	05/1997	Mohanty *et al.*	395	326	
AM	AJ3	5,635,598	06/1997	Lebl *et al.*	530	334	
AM	AK3	5,670,326	09/1997	Beutel	435	7.1	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
AM	AL3	WO 97/20952	06/1997	PCT, Pakula et al.	C12Q	1/68	Yes No
AM	AM3	WO 97/27559	07/1997	PCT, Patterson et al.	G06F	19/00	Yes No
AM	AN3	WO 98/20437	05/1998	PCT, Agrafiotis et al.	G06F	17/50	Yes No
AM	AO3	WO 98/20459	05/1998	PCT, Agrafiotis et al.	G06T	11/20	Yes No
	AP3						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	3	Andrea, T.A. *et al.*, "Applications of Neural Networks in Quantitative Structure-Activity Relationships of Dihydrofolate Reductase Inhibitors," *Journal of Medicinal Chemistry*," Vol. 34, No. 9, pp. 2824-2836, (1991).
AM	AS	3	Aoyama, T. *et al.*, "Neural Networks Applied to Quantitative Structure-Activity Relationship Analysis," *Journal of Medicinal Chemistry*, Vol. 33, No. 9, pp. 2583-2590, (1990).
AM	AT	3	Aoyama, T. *et al.*, "Neural Networks Applied to Structure-Activity Relationships," *Journal of Medicinal Chemistry*, Vol. 33, No. 3, pp. 905-908, (1990).

EXAMINER Andrew Marsden	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AM	AA4	5,679,582	10/1997	Bowie *et al.*	436	518	
AM	AB4	5,684,711	11/1997	Agrafiotis *et al.*	364	500	
AM	AC4	5,703,792	12/1997	Chapman	364	496	
AM	AD4	5,712,171	01/1998	Zambias *et al.*	436	518	
AM	AE4	5,712,564	01/1998	Hayosh	324	210	
AM	AF4	5,736,412	04/1998	Zambias *et al.*	436	518	
AM	AG4	5,789,160	08/1998	Eaton *et al.*	435	6	
AM	AH4	5,807,754	09/1998	Zambias *et al.*	436	518	
AM	AI4	5,811,241	09/1998	Goodfellow *et al.*	435	7.1	
AM	AJ4	5,832,494	11/1998	Egger *et al.*	707	102	
AM	AK4	5,858,660	01/1999	Eaton *et al.*	435	6	

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL4						Yes No
	AM4						Yes No
	AN4						Yes No
	AO4						Yes No
	AP4						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	4	Aoyama, T. and Hiroshi Ichikawa, "Obtaining the Correlation Indices between Drug Activity and Structural Parameters Using a Neural Network," *Chemical & Pharmaceutical Bulletin*, Vol. 39, No. 2, pp. 372-378, (1991).
AM	AS	4	"ArQule Inc," from http://www.bioportfolio.com/arqule/products.htm, 5 pages, (March 18, 1998).
AM	AT	4	Baum, R.M., "Combinatorial Approaches Provide Fresh Leads for Medicinal Chemistry," *Chemical & Engineering News*, February 7, 1994 (pp. 20-26).

EXAMINER	Andrew Marschel	DATE CONSIDERED	9/23/02

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AM	AA5	5,861,532	01/1999	Brown *et al.*	564	142	
AM	AB5	5,866,334	02/1999	Beutel	435	6	
AM	AC5	5,901,069	05/1999	Agrafiotis *et al.*	364	528.03	
AM	AD5	5,908,960	06/1999	Newlander	564	177	
AM	AE5	5,933,819	08/1999	Skolnick *et al.*	706	21	
AM	AF5	6,037,135	03/2000	Kubo *et al.*	435	7.24	
AM	AG5	6,049,797	04/2000	Guha *et al.*	707	6	
	AH5						
	AI5						
	AJ5						
	AK5						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL5						Yes No
	AM5						Yes No
	AN5						Yes No
	AO5						Yes No
	AP5						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	5	Bentley, J.L., "Multidimensional Binary Search Trees Used for Associative Searching," *Communications of the ACM*, Vol. 18, No. 9, pp. 509-517, (September 1975).
AM	AS	5	Blaney, J.M. and Martin, E.J., "Computational approaches for combinatorial library design and molecular diversity analysis," *Current Opinion in Chemical Biology*, Vol. 1, No. 1, June 1997, pp. 54-59.
AM	AT	5	Bottou, L. and Vladimir Vapnik, "Local Learning Algorithms," *Neural Computation*, Vol. 4, No. 6, pp. 888-900, (November 1992).

EXAMINER	Andrew Mansfield	DATE CONSIDERED	9/23/02

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA6						
	AB6						
	AC6						
	AD6						
	AE6						
	AF6						
	AG6						
	AH6						
	AI6						
	AJ6						
	AK6						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL6						Yes No
	AM6						Yes No
	AN6						Yes No
	AO6						Yes No
	AP6						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	6	Boulu, L.G. and Gordon M. Crippen, "Voronoi Binding Site Models: Calculation of Binding Modes and Influence of Drug Binding Data Accuracy," *Journal of Computational Chemistry*, Vol. 10, No. 5, pp. 673-682, (1989).
AM	AS	6	Boulu, L.G. *et al.*, "Voronoi Binding Site Model of a Polycyclic Aromatic Hydrocarbon Binding Protein," *Journal of Medicinal Chemistry*, Vol. 33, No. 2, pp. 771-775, (1990).
AM	AT	6	Brown, R.D. and Clark, D.E., "Genetic Diversity: Applications of evolutionary algorithms to combinatorial library design," *Expert Opinion on Therapeutic Patents*, Vol. 8, No. 11, November 1998, pp. 1447-1459.

EXAMINER Sardis Massey	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA7						
	AB7						
	AC7						
	AD7						
	AE7						
	AF7						
	AG7						
	AH7						
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	AJ7						
	AK7						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL7						Yes No
	AM7						Yes No
	AN7						Yes No
	AO7						Yes No
	AP7						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	7	Brown, R.D. and Yvonne C. Martin, "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection," *Journal of Chemical Information and Computer Sciences*, Vol. 36, No. 3, pp. 572-584, (1996).
AM	AS	7	Cacoullos, T., "Estimation of a Multivariate Density", *Annals of The Institute of Statistical Mathematics*, Vol. 18, No. 2, pp. 179-189, (1966).
AM	AT	7	Caflisch, A. and Karplus, M., "Computational combinatorial chemistry for de novo ligand design: Review and assessment," Perspectives in Drug Discovery and Design, Vol. 3, 1995, pp. 51-84.

EXAMINER	Andrew Massey	DATE CONSIDERED	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA8						
	AB8						
	AC8						
	AD8						
	AE8						
	AF8						
	AG8						
	AH8						
	AI8						
	AJ8						
	AK8						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL8						Yes No
	AM8						Yes No
	AN8						Yes No
	AO8						Yes No
	AP8						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	8	Clark, D. E., and David R. Westhead, "Evolutionary algorithms in computer-aided molecular design", *Journal of Computer-Aided Molecular Design*, Vol. 10, No. 4, pp. 337-358, (August 1996).
AM	AS	8	Clark, R.D., "OptiSim: An Extended Dissimilarity Selection Method for Finding Diverse Representative Subsets", *Journal of Chemical Information and Computer Sciences*, Vol. 37, No. 6, pp. 1181-1188 (*12 Page Internet printout*), 1997.
AM	AT	8	Cramer, R. D. III *et al.*, "Comparative Molecular Field Analyisis (CoMFA). 1. Effect of Shape on Binding of Steroids to Carrier Proteins", *Journal of The American Chemical Society*, Vol. 110, No. 18, pp. 5959-5967, (August 31, 1988).

EXAMINER Andrew Mansfield	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA9						
	AB9						
	AC9						
	AD9						
	AE9						
	AF9						
	AG9						
	AH9						
	AI9						
	AJ9						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL9						Yes No
	AM9						Yes No
	AN9						Yes No
	AO9						Yes No
	AP9						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	9	Cramer, R. D. III *et al.*, "Substructural Analysis. A Novel Approach to the Problem of Drug Design", *Journal of Medicinal Chemistry*, Vol. 17, No. 5, pp. 533-535, (May 1974).
AM	AS	9	Crippen, G. M., "Voronoi binding Site Models", *Journal of Computational Chemistry*, Vol. 8, No. 7, pp. 943-955, (October/November 1987).
AM	AT	9	Danheiser, S.L., "Current Trends in Synthetic Peptide and Chemical Diversity Library Design," *Genetic Engineering News*, May 1, 1994, pp. 10 and 31.

EXAMINER Andrew Marschke — DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA10						
	AB10						
	AC10						
	AD10						
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	AH10						
	AI10						
	AJ10						
	AK10						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL10						Yes No
	AM10						Yes No
	AN10						Yes No
	AO10						Yes No
	AP10						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	10	Eichler, U. *et al.*, "Addressing the problem of molecular diversity," *Drugs of the Future*, Vol. 24, No. 2, 1999, pp. 177-190.
AM	AS	10	Felder, E.R. and Poppinger, D., "Combinatorial Compound Libraries for Enhanced Drug Discovery Approaches," Advances in Drug Research, Vol. 30, 1997, pp. 112-199.
AM	AT	10	Friedman, J. H. *et al.*, "An Algorithm for Finding Best Matches in Logarithmic Expected Time", *ACM Transactions on Mathematical Software*, Vol. 3, No. 3, pp. 209-226, (September 1977).

EXAMINER	Audin Marshall	DATE CONSIDERED	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA11						
	AB11						
	AC11						
	AD11						
	AE11						
	AF11						
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	AH11						
	AI11						
	AJ11						
	AK11						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL11						Yes No
	AM11						Yes No
	AN11						Yes No
	AO11						Yes No
	AP11						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	11	Friedman, J.H., "Fitting Functions To Noisy Data In High Dimensions", Department of Statistics- Stanford University Technical Report No. 101, (August, 1988).
AM	AS	11	Gallop, M. A. *et al.*, "Applications of Combinatorial Technologies to Drug Discovery. 1. Background and Peptide Combinatorial Libraries", *Journal of Medicinal Chemistry*, Vol. 37, No. 9, pp. 1233-1251, (April 29, 1994).
AM	AT	11	Geysen, H.M. and Mason, T.J., "Screening Chemically Synthesized Peptide Libraries for Biologically-Relevant Molecules," *Biorganic & Medicinal Chemistry Letters*, Vol. 3, No. 3, 1993, pp. 397-404.

EXAMINER	DATE CONSIDERED
Lydia Mason	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA12						
	AB12						
	AC12						
	AD12						
	AE12						
	AF12						
	AG12						
	AH12						
	AI12						
	AJ12						
	AK12						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL12						Yes No
	AM12						Yes No
	AN12						Yes No
	AO12						Yes No
	AP12						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	12	Ghose, A. K. and Gordon M. Crippen, "Use of Physicochemical Parameters in Distance Geometry and Related Three-Dimensional Qantitative Structure-Activity Relationships: A Demonstration Using *Escherichia coli* Dihydrofolate Reductase Inhibitors", *Journal of Medicinal Chemistry*, Vol. 28, No. 3, pp. 333-346, (1985).
AM	AS	12	Gobbi, A. *et al.*, "New Leads By Selective Screening of Compounds From Large Databases," *Abstracts for CINF sponsored symposia*, April 17, 1997, p. 22.
AM	AT	12	Good, A. C. *et al.*, "Structure-Activity Relationships from Molecular Similarity Matrices", *Journal of Medicinal Chemistry*, Vol. 36, No. 4, pp. 433-438, (February 19, 1993).

EXAMINER	Audrey Macsley	DATE CONSIDERED	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA13						
	AB13						
	AC13						
	AD13						
	AE13						
	AF13						
	AG13						
	AH13						
	AI13						
	AJ13						
	AK13						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL13						Yes No
	AM13						Yes No
	AN13						Yes No
	AO13						Yes No
	AP13						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	13	Gordon, E. M., "Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic Synthesis, Library Screening Strategies, and Future Directions", *Journal of Medicinal Chemistry*, Vol. 37, No. 10, (May 13, 1994).
AM	AS	13	Grayhill, T.L. *et al.*, "Enhancing the Drug Discovery Process by Integration of High-Throughput Chemistry and Structure-Based Drug Design," from Molecular Diversity and Combinatorial Chemistry: Libraries and Drug Discovery, Chaiken and Janda (eds.), American Chemical Society, 1996, pp. 16-27.
AM	AT	13	Hartigan, J. A., "Representation of Similarity Matrices By Trees", *Journal of the American Statistical Association*, Vol. 62, No. 320, pp. 1140-1158, (December, 1967).

EXAMINER	Andrew Marschel	DATE CONSIDERED	9/23/02

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FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA14						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL14						Yes No
	AM14						Yes No
	AN14						Yes No
	AO14						Yes No
	AP14						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	14	Hopfinger, A. J., "A QSAR Investigation of Dihydrofolate Reductase Inhibition by Baker Triazines based upon Molecular Shape Analysis", *Journal of the American Chemical Society*, Vol. 102, No. 24, pp. 7196-7206, (November 19, 1980).
AM	AS	14	Houghten, R.A. *et al.*, "The Use of Synthetic Peptide Combinatorial Libraries for the Identification of Bioactive Peptides," *Peptide Research*, Vol. 5, No. 6, 1992, pp. 351-358.
AM	AT	14	Jackson, R. C., "Update on computer-aided drug design", *Current Opinion in BIOTECHNOLOGY*, Vol. 6, No. 6, pp. 646-651, (December, 1995).

EXAMINER	DATE CONSIDERED
Andrew Marschel	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA15						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL15						Yes No
	AM15						Yes No
	AN15						Yes No
	AO15						Yes No
	AP15						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	15	Kim, K. H., "Comparative molecular field analysis (CoFMA)", Molecular Similarity in Drug Design, ed. P. M. Dean, Blackie Academic & Professional, 1995, Ch. 12 (pp. 291-324).
AM	AS	15	Klopman, G., "Artificial Intelligence Approach to Structure-Activity Studies. Computer Automated Structure Evaluation of Biological Activity of Organic Molecules," *J. Am. Chem. Soc.*, Vol. 106, No. 24, November 28, 1984, pp. 7315-7321.
AM	AT	15	Kohonen, T., "Self-Organized Formation of Topologically Correct Feature Maps", *Biological Cybernetics*, Vol. 43, pp. 59-69, (1982).

EXAMINER Andrea Mansfield	DATE CONSIDERED 9/23/02

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FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA16						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL16						Yes No
	AM16						Yes No
	AN16						Yes No
	AO16						Yes No
	AP16						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	16	Koile, K. and Richard Shapiro, "Building A Collaborative Drug Design System", *Proceedings of the 25h Hawaii International Conference on System Sciences*, pp. 706-716, (1992).
AM	AS	16	Kowalski, B. R. and C. F. Bender, "Pattern Recognition. II. Linear and Nonlinear Methods for Displaying Chemical Data", *Journal of the American Chemical Society*, pp. 686-693, (February 7, 1973).
AM	AT	16	Kruskal, J. B., "Nonmetric Multidimensional Scaling: A Numerical Method", *Psychometrika*, Vol. 29, No. 2, pp. 115-129, (June, 1964).

EXAMINER Andrea Mansley — DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA17						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL17						Yes No
	AM17						Yes No
	AN17						Yes No
	AO17						Yes No
	AP17						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	17	Lajiness, M.S. *et al.*, "Implementing Drug Screening Programs Using Molecular Similarity Methods," QSAR: Quantitative Structure-Activity Relationships in Drug Design, 1989, pp. 173-176.
AM	AS	17	Lengauer, T. and Matthias Rarey, "Computational methods for biomolecular docking", *Current Opinion in Structural Biology*, Vol. 6, No. 3, pp. 402-406, (June, 1996).
AM	AT	17	Loew, G.H. *et al.*, "Strategies for Indirect Computer-Aided Drug Design," *Pharmaceutical Research*, Vol. 10, No. 4, 1993, pp. 475-486.

EXAMINER Adin Mascot	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL18						Yes No
	AM18						Yes No
	AN18						Yes No
	AO18						Yes No
	AP18						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	18	Luke, B. T., "Evolutionary Programming Applied to the Development of Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences*, Vol. 34, pp. 1279-1287, (November/December, 1994).
AM	AS	18	Lynch, M.F. *et al.*, "Generic Structure Storage and Retrieval," *J. Chem. Inf. Comput. Sci.*, Vol. 25, No. 3, August 1985, pp. 264-270.
AM	AT	18	Martin, E. J. *et al.*, "Does Combinatorial Chemistry Obviate Computer-Aided Drug Design?", *Reviews in Computational Chemistry*, Vol. 10, pp. 75-99, (1997).

EXAMINER Andrew Marasley	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA19						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL19						Yes No
	AM19						Yes No
	AN19						Yes No
	AO19						Yes No
	AP19						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	19	Martin, E. J. *et al.*, "Measuring Diversity: Experimental Design of Combinatorial Libraries for Drug Discovery", *Journal of Medicinal Chemistry*, Vol. 38, No. 9, pp. 1431-1436, (April 28, 1995).
AM	AS	19	McMartin, C. and Regine S. Bohacek, "QXP: Powerful, rapid computer algorithms for structure-based drug design", *Journal of Computer-Aided Molecular Design*, Vol. 11, pp. 333-344, (1997).
AM	AT	19	Mezey, P. G. and P. Duane Walker, "Fuzzy molecular fragments in drug research", *Drug Discovery Today*, Vol. 2, No. 4, (April, 1997).

EXAMINER Andi Mauser	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA20						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL20						Yes No
	AM20						Yes No
	AN20						Yes No
	AO20						Yes No
	AP20						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

DM	AR	20	Müller, K., "On the paradigm shift from rational to random design", *Journal of Molecular Structure (Theochem)398-399*, Special Issue, pp. 467-471, (1997).
	AS	20	~~Myers, P., "The Design Of A Universal, Informer™ Library", COMBICHEM, INC., 10 Pages, Date unknown.~~
DM	AT	20	Myers, P.L. *et al.*, "Rapid, Reliable Drug Discovery," *Today's Chemist At Work*, July/August 1997, pp. 46-48, 51 & 53.

EXAMINER	Andrea Marshall	DATE CONSIDERED	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL21						Yes No
	AM21						Yes No
	AN21						Yes No
	AO21						Yes No
	AP21						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	~~AR~~	~~21~~	~~Omohundro, S. M., "Bumptrees for Efficient Function, Constraint, and Classification Learning", International Computer Science Institute, pp. 693-699, Source and Date unknown.~~
AM	AS	21	Pabo *et al.*, "Computer-Aided Model Building Strategies for Protein Design," *Biochemistry*, Vol. 25, No. 20, 1986, pp. 5987-5991.
AM	AT	21	Parrill, A. L., "Evolutionary and genetic methods in drug design", *Drug Discovery Today*, Vol. 1, No. 12, pp. 514-521, (December, 1996).

EXAMINER Dudin Mansdorf — DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA22						
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL22						Yes No
	AM22						Yes No
	AN22						Yes No
	AO22						Yes No
	AP22						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	22	Polanski, J., "A neural network for the simulation of biological systems", *Journal of Molecular Structure (Theochem)398-399*, Special Issue, pp. 565-571, (1997).
AM	AS	22	Ramos-Nino, M. E. *et al.*, "A comparison of quantitative structure-activity relationships for the effect of benzoic and cinnamic acids on *Listeria monocytogenes* using multiple linear regression, artificial neural network and fuzzy systems", *Journal of Applied Microbiology*, Vol. 82, No. 2, pp. 168-175, (February, 1997).
AM	AT	22	Rogers, D. and A. J. Hopfinger, "Application of Genetic Function Approximation to Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships", *Journal of Chemical Information and Computer Sciences*, Vol. 34, No. 4, pp. 854-866, (July/August, 1994).

EXAMINER Andrew Mazdy	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA23						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL23						Yes No
	AM23						Yes No
	AN23						Yes No
	AO23						Yes No
	AP23						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	23	Sammon, J. W., Jr., "A Nonlinear Mapping for Data Structure Analysis", *IEEE Transactions on Computers*, Vol. C-18, No. 5, pp. 401-409, (May, 1969).
AM	AS	23	Saudek *et al.*, "Solution Conformation of Endothelin-1 by H NMR, CD, and Molecular Modeling," *International Journal of Peptide Protein Res.*, Vol. 37, No. 3, 1991, pp. 174-179.
AM	AT	23	Saund, E., "Dimensionality-Reduction Using Connectionist Networks," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, Vol. 11, No. 3, March 1989, pp. 304-314.

EXAMINER Andrei Manacher DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA24						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL24						Yes No
	AM24						Yes No
	AN24						Yes No
	AO24						Yes No
	AP24						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	24	Simon, Z. *et al.*, "Mapping of Dihydrofolate-reductase Receptor Site by Correlation with Minimal Topological (Steric) Differences", *Journal of Theoretical Biology*, Vol. 66, No. 3, pp. 485-495, (June 7, 1997).
AM	AS	24	Singh, J. *et al.*, "Application of Genetic Algorithms to Combinatorial Synthesis: A Computational Approach to Lead Identification and Lead Optimization," *J. Am. Chem. Soc.*, Vol. 118, No. 7, February 21, 1996, pp. 1669-1676.
AM	AT	24	Smellie, A. S. *et al.*, "Fast Drug-Receptor Mapping by Site-Directed Distances: A Novel Method of Predicting New Pharmacological Leads", *Journal of Chemical Information and Computer Sciences*, Vol. 31, No.3, pp. 386-392, (August, 1991).

EXAMINER Andrei Manolov — DATE CONSIDERED 9/23/02

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	AA25						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL25						Yes No
	AM25						Yes No
	AN25						Yes No
	AO25						Yes No
	AP25						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	25	Specht, D. F., "A General Regression Neural Network", *IEEE Transactions on Neural Networks*, Vol. 2, No. 6, pp. 568-576, (November, 1991).
AM	AS	25	Svozil, D. *et al.*, "Neural Network Prediction of the Solvatochromic Polarity/Polarizability Parameter π^{H}_{2}", *Journal of Chemical Information and Computer Sciences*, Vol. 37, No. 2, (1997).
AM	AT	25	Todorov, N. P. and P. M. Dean, "Evaluation of a method for controlling molecular scaffold diversity in de novo ligand design", *Journal of Computer-Aided Molecular Design*, Vol. 11, pp. 175-192, (1997).

EXAMINER Andrew Massaden DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA26						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL26						Yes No
	AM26						Yes No
	AN26						Yes No
	AO26						Yes No
	AP26						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	26	Torgerson, W. S., "Multidimensional Scaling: I. Theory and Method", *Psychometrika*, Vol. 17, No. 4, pp. 401-419, (December, 1952).
AM	AS	26	Van Drie, J.H. and Lajiness, M.S., "Approaches to virtual library design," *Drug Discovery today*, Vol. 3, No. 6, June 1998, pp. 274-283.
AM	AT	26	Vapnik, V. and L. Bottou, "Local Algorithms for Pattern Recognition and Dependencies Estimation", *Neural Computation*, Vol. 5, No. 6, pp. 893-909, (November, 1993).

EXAMINER Andrew Monaden	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA27						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL27						Yes No
	AM27						Yes No
	AN27						Yes No
	AO27						Yes No
	AP27						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	AR	27	~~Vapnik, V., "Principles of Risk Minimization for Learning Theory", *Advances in Neural Information Processing Systems 4*, pp. 831-838, Date unknown.~~
AM	AS	27	Viswanadhan, V. N. *et al.*, "Mapping the binding site of the nucleoside transporter protein: a 3D-QSAR study", *Biochimica et Biophysica Acta*, Vol. 1039, No. 3, pp. 356-366, (1990).
AM	AT	27	Walters, W.P., "Virtual screening - an overview," *Drug Discovery today*, Vol. 3, No. 4, April 1998, pp. 160-178.

EXAMINER Andrew Marshall DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA28						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL28						Yes No
	AM28						Yes No
	AN28						Yes No
	AO28						Yes No
	AP28						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	28	Warr, W. A., "Exploiting Molecular Diversity: Small Molecule Libraries for Drug Discovery", Report of Conference held in La Jolla, California, Jan. 23-25, 1995.
AM	AS	28	Weber, L., "Evolutionary combinatorial chemistry: application of genetic algorithms," *Drug Discovery today*, Vol. 3, No. 8, August 1998, pp. 379-385.
AM	AT	28	Weber, L. *et al.*, "Optimization of the Biological Activity of Combinatorial Compound Libraries by a Genetic Algorithm," *Angewandte Chemie International Edition in English*, Vol. 34, No. 20, 1995, pp. 2280-2282.

EXAMINER Andrew Marcley — DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA29						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL29						Yes No
	AM29						Yes No
	AN29						Yes No
	AO29						Yes No
	AP29						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	29	Westhead, D. R. *et al.*, "A comparison of heuristic search algorithms for molecular docking", *Journal of Computer-Aided Molecular Design*, Vol. 11, pp. 209-228, (1997).
AM	AS	29	Willett, P., "Genetic algorithms in molecular recognition and design", *Trends in Biotechnology*, Vol, 13, No. 12, pp. 516-521, (December, 1995).
AM	AT	29	Willett, P. and Vivienne Winterman, "A Comparison of Some Measures for the Determination of Inter-Molecular Structural Similarity Measures of Inter-Molecular Structural Similarity", *Quantitative Structure-Activity Relationships*, Vol. 5, No. 1, pp. 18-25, (March, 1986).

EXAMINER Andrew Marshall	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL30						Yes No
	AM30						Yes No
	AN30						Yes No
	AO30						Yes No
	AP30						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	30	Zadeh, L. A., "Communication Fuzzy Algorithms", *Information and Control*, Vol. 12, No. 2, pp. 94-102, (February, 1968).
AM	AS	30	Zadeh, L. A., "Fuzzy Sets", *Information and Control*, Vol. 8, No. 3, pp. 338-353, (June, 1965).
AM	AT	30	Borg, Inger and Groenen, Patrick, *Modern Multidimensional Scaling Theory and Applications*, Springer Series in Statistics, 1997, entire book submitted.

EXAMINER Andrew Massaby	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL31						Yes No
	AM31						Yes No
	AN31						Yes No
	AO31						Yes No
	AP31						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	31	Agrafiotis, D.K. *et al.*, "Advances in diversity profiling and combinatorial series design," *Molecular Diversity*, Vol. 4, 1999, pp. 1-22.
AM	AS	31	Agrafiotis, D.K. and Lobanov, V.S., "An Efficient Implementation of Distance-Based Diveristy Measure based on *k-d* Trees," *J. Chem. Inf. Comput. Sci.*, Vol. 39, No. 1, January/February 1999, pp. 51-58.
AM	AT	31	Agrafiotis, D.K. and Lobanov, V.S., "Bridging The Gap Between Diversity And QSAR," *Abstracts of Papers Part 1: 215th ACS National Meeting*, March 29-April 2, 1998, p. 181-COMP.

EXAMINER Andrew Marschke	DATE CONSIDERED 9-23-02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL32						Yes No
	AM32						Yes No
	AN32						Yes No
	AO32						Yes No
	AP32						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

DM	AR	32	Agrafiotis, D.K. and Jaeger, E.P., "Directed Diversity®: An Operating System For Combinatorial Chemistry," *Abstracts of Papers Part 1: 211th ACS National Meeting*, March 24-28, 1996, p. 46-COMP.
DM	AS	32	Agrafiotis, D.K., "Diversity of Chemical Libraries," *Encyclopedia of Computational Chemistry*, Vol. 1:A-D, 1998, pp. 742-761.
DM	AT	32	Agrafiotis, D.K., "On the Use of Information Theory for Assessing Molecular Diversity," *J. Chem. Inf. Comput. Sci.*, Vol. 37, No. 3, May/June 1997, pp. 576-580.

EXAMINER	Sidney Morschel	DATE CONSIDERED	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL33						Yes No
	AM33						Yes No
	AN33						Yes No
	AO33						Yes No
	AP33						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	33	Agrafiotis, D.K. *et al.*, "Parallel QSAR," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 50-COMP.
AM	AS	33	Agrafiotis, D.K. *et al.*, "PRODEN: A New Program for Calculating Integrated Projected Populations," *Journal of Computational Chemistry*, Vol. 11, No. 9, October 1990, pp. 1101-1110.
AM	AT	33	Agrafiotis, D.K. and Jaeger, E.P., "Stochastic Algorithms for Exploring Molecular Diversity," *Abstracts of Papers Part 1: 213th ACS National Meeting*, April 13-17, 1997, p. 16-CINF.

EXAMINER Andrew Marsden DATE CONSIDERED 9/23/02

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL34						Yes No
	AM34						Yes No
	AN34						Yes No
	AO34						Yes No
	AP34						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	34	Agrafiotis, D., "Theoretical Aspects of the Complex: Arts and New Technologies," *Applications and Impacts Information Processing '94*, Vol. II, 1994, pp. 714-719.
AM	AS	34	Biswas, G. *et al.*, "Evaluation of Projection Algorithms," *IEEE Transactions On Pattern Analysis And Machine Intelligence*, Vol. PAMI-3, No. 6, November 1981, pp. 701-708.
AM	AT	34	Bonchev, D. and Trinajsti, N., "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, Vol. 67, No. 10, November 15, 1977, pp. 4517-4533.

EXAMINER Adam Marschel DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL35						Yes No
	AM35						Yes No
	AN35						Yes No
	AO35						Yes No
	AP35						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	35	Chang, C.L. and Lee, R.C.T., "A Heuristic Relaxation Method for Nonlinear Mapping in Cluster Analysis," *IEEE Transactions on Systems, Man, and Cybernetics*, Vol. SMC-3, March 1973, pp. 197-200.
AM	AS	35	Cramer, R.D. *et al.*, "Virtual Compound Libraries: A New Approach to Decision Making in Molecular Discovery Research," *J. Chem. Inf. Comput. Sci.*, Vol. 38, No. 6, November/December 1998, pp. 1010-1023.
AM	AT	35	DeMers, D. and Cottrell, G., "Non-Linear Dimensionality Reduction," *Advances in Neural Information Processing Systems*, Vol. 5, 1993, pp. 580-587.

EXAMINER Andrew Mansfield — DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA36						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL36						Yes No
	AM36						Yes No
	AN36						Yes No
	AO36						Yes No
	AP36						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	36	Frey, P.W. and Slate, D.J., "Letter Recognition Using Holland-Style Adaptive Classifiers," *Machine Learning*, Vol. 6, 1991, pp. 161-182.
AM	AS	36	Friedman, J.H., "Exploratory Projection Pursuit," *Journal of the American Statistical Association*, Vol. 82, No. 397, March 1987, pp. 249-266.
AM	AT	36	Friedman, J.H. and Tukey, J.W., "A Projection Pursuit Algorithm for Exploratory Data Analysis," *IEEE Transactions on Computers*, Vol. C-23, No. 9, September 1974, pp. 881-889.

EXAMINER Andrew Marschel	DATE CONSIDERED 9/23/02

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL37						Yes No
	AM37						Yes No
	AN37						Yes No
	AO37						Yes No
	AP37						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	37	Garrido, L. *et al.*, "Use of Multilayer Feedforward Neural Nets As A Display Method for Multidimensional Distributions," *International Journal of Neural Systems*, Vol. 6, No. 3, September 1995, pp. 273-282.
AM	AS	37	Ghose, A.K. *et al.*, "Prediction of Hydrophobic (Lipophilic) Properties of Small Organic Molecules Using Fragmental Methods: An Analysis of ALOGP and CLOGP Methods," *J. Phys. Chem. A*, Vol. 102, No. 21, May 21, 1998, pp. 3762-3772.
AM	AT	37	Hall, L.H. and Kier, L.B., "The Molecular Connectivity Chi Indexes and Kappa Shape Indexes in Structure-Property Modeling," *Reviews in Computational Chemistry: Advances*, 1991, pp. 367-422.

EXAMINER Jordan Marschel	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA38						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL38						Yes No
	AM38						Yes No
	AN38						Yes No
	AO38						Yes No
	AP38						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	38	Hecht-Nielsen, R., "Replicator Neural Networks for Universal Optimal Source Coding," *Science*, Vol. 269, September 29, 1995, pp. 1860-1863.
AM	AS	38	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Vol. XXIV, No. 6, September 1933, pp. 417-441.
AM	AT	38	Hotelling, H., "Analysis of a Complex of Statistical Variables into Principal Components," *The Journal of Educational Psychology*, Vol. XXIV, No. 7, October 1933, pp. 498-520.

EXAMINER Julian Mercedel	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL39						Yes No
	AM39						Yes No
	AN39						Yes No
	AO39						Yes No
	AP39						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	39	Lee, R.C.T. *et al.*, "A Triangulation Method for the Sequential Mapping of Points from *N*-Space to Two-Space," *IEEE Transactions on Computers*, March 1977, pp. 288-292.
AM	AS	39	Lipinski, C.A. *et al.*, "Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings," *Advanced Drug Delivery Reviews*, Vol. 23, 1997, pp. 3-25.
AM	AT	39	Lobanov, V.S. and Agrafiotis, D.K., "Intelligent Database Mining Techniques," *Abstracts of Papers Part 1: 215th ACS National Meeting*, March 29-April 2, 1998, p. 19-COMP.

EXAMINER Andrew Marucci	DATE CONSIDERED 9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL40						Yes No
	AM40						Yes No
	AN40						Yes No
	AO40						Yes No
	AP40						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	40	Lobanov, V.S. *et al.*, "Rational Selections from Virtual Libraries," *Abstracts of Papers Part 1: 217th ACS National Meeting*, March 21-25, 1999, p. 181-COMP.
AM	AS	40	Mao, J. and Jain, A.K., "Artificial Neural Networks for Feature Extraction and Multivariate Data Projection," *IEEE transactions on Neural Networks*, Vol. 6, No. 2, March 1995, pp. 296-317.
AM	AT	40	Oja, E., "Principal Components, Minor Components, and Linear Neural Networks," *Neural Networks*, Vol. 5, 1992, pp. 927-935.

EXAMINER	Andrew Marschel	DATE CONSIDERED	9/23/02

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL41						Yes No
	AM41						Yes No
	AN41						Yes No
	AO41						Yes No
	AP41						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	41	Patterson, D.E. *et al.*, "Neighborhood Behavior: A Useful Concept for Validation of 'Molecular Diversity' Descriptors," *Journal of Medicinal Chemistry*, Vol. 39, No. 16, 1996, pp. 3049-3059.
AM	AS	41	Pykett, C.E., "Improving the Efficiency of Sammon's Nonlinear Mapping by Using Clustering Archetypes," *Electronics Letters*, Vol. 14, No. 25, December 7, 1978, pp. 799-800.
AM	AT	41	Rubner, J. and Tavan, P., "A Self-Organizing Network for Principal-Component Analysis," *Europhysics Letters*, Vol. 10, No. 7, December 1, 1989, pp. 693-698.

EXAMINER Andrew Mansfield	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL42						Yes No
	AM42						Yes No
	AN42						Yes No
	AO42						Yes No
	AP42						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	42	Sadowski, J. *et al.*, "Assessing Similarity and Diversity of Combinatorial Libraries by Spatial Autocorrelation Functions and Neural Networks," *Angewandte Cheme*, Vol. 34, No. 23/24, January 5, 1996, pp. 2674-2677.
AM	AS	42	Thompson, L.A. and Ellman, J.A., "Synthesis and Applications of Small Molecule Libraries," *Chemical Reviews*, Vol. 96, No. 1, January/February 1996, pp. 555-600.
AM	AT	42	Barnard, John M. and Downs, Geoff M., "Computer representation and manipulation of combinatorial libraries," *Perspectives in Drug Discovery and Design*, 1997, pp. 13-30.

EXAMINER Ardin Marschel	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL43						Yes No
	AM43						Yes No
	AN43						Yes No
	AO43						Yes No
	AP43						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	43	Brint, Andrew T. and Willett, Peter, "Upperbound procedures for the identification of similar three-dimensional chemical structures," *Journal of Computer-Aided Molecular Design*, Vol. 2, No. 4, 1988, pp. 311-320.
AM	AS	43	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," *Journal of Medicinal Chemistry*, Vol. 40, No. 15, 1997, pp. 2304-2313.
AM	AT	43	Gasteiger, J. *et al.*, "Analysis of the Reactivity of Single Bonds in Aliphatic Molecules by Statistical and Pattern Recognition Methods," *Journal of Chemical Information Computer Science*, Vol. 33, No. 3, 1993, pp. 385-394.

EXAMINER Andrea Marschke	DATE CONSIDERED 9/23/02

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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL44						Yes No
	AM44						Yes No
	AN44						Yes No
	AO44						Yes No
	AP44						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	44	Gillet, Valerie J. *et al.*, "The Effectiveness of Reactant Pools for Generating Structurally-Diverse Combinatorial Libraries," *Journal of Chemical Information Computer Sciences*, Vol. 37, No. 4, 1997, pp. 731-740.
AM	AS	44	Gillet, Valerie J. *et al.*, "Selecting Combinatorial Libraries to Optimize Diversity and Physical Properties," *Journal of Chemical Information Computer Sciences*, Vol. 39, No. 1, 1999, pp. 169-177.
AM	AT	44	Guez, Allon and Nevo, Igal, "Neural networks and fuzzy logic in clinical laboratory computing with application to integrated monitoring," *Clinica Chimica Acta*, 248, 1996, pp. 73-90.

EXAMINER Andrew Mansfield DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA45						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL45						Yes No
	AM45						Yes No
	AN45						Yes No
	AO45						Yes No
	AP45						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	45	Kearsley, Simon K. *et al.*, "Chemical Similarity Using Physiochemical Property Descriptors," *Journal of Chemical Information Computer Science*, 36, 1996, pp. 118-127.
AM	AS	45	Leland, Burton A. *et al.*, "Managing the Combinatorial Explosion," *Journal of Chemical Information Computer Science*, 37, 1997, pp. 62-70.
AM	AT	45	Lewis, Richard A. *et al.*, "Similarity Measures for Rational Set Selection and Analysis of Combinatorial Libraries: The Diverse Property-Derived (DPD) Approach," *Journal of Chemical Information Computer Science*, 37, 1997, pp. 599-614.

EXAMINER Andi Masley DATE CONSIDERED 9/23/02

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	APPLICANT Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA46						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL46						Yes No
	AM46						Yes No
	AN46						Yes No
	AO46						Yes No
	AP46						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	46	Martin, Eric J. and Critchlow, Roger E., "Beyond Mere Diversity: Tailoring Combinatorial Libraries for Drug Discovery," *Journal of Combinatorial Chemistry*, Vol. 1, No. 1, 1999, pp. 32-45.
AM	AS	46	Sen, K. (ed.), *Molecular Similarity I*, Springer-Verlag, 1995, pp. 1-30.
AM	AT	46	Sheridan, Robert P. *et al.*, "Chemical Similarity Using Geometric Atom Pair Descriptors," *Journal of Chemical Information Computer Science*, 36, 1996, pp. 128-136.

EXAMINER Austin Mazaley DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA47						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL47						Yes No
	AM47						Yes No
	AN47						Yes No
	AO47						Yes No
	AP47						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	47	Willett, Peter *et al.*, "Chemical Similarity Searching," *Journal of Chemical Information Computer Science*, 38, 1998, pp. 983-996.
AM	AS	47	Agrafiotis, Dimitris K. and Lobanov, Victor S., "Ultrafast Algorithm for Designing Focused Combinational Arrays," *J. Chem. Inf. Comput. Sci.*, June 16, 2000, Vol. 40, pp. 1030-1038.
AM	AT	47	Ajay, W. Patrick Walters and Murcko, Mark A., "Can We Learn To Distinguish between "Drug-Like" and "Nondrug-like" Molecules?" *J. Med. Chem.*, July 23, 1998, Vol. 41, pp. 3314-3324.

EXAMINER Andrew Massefski	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA48						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL48						Yes No
	AM48						Yes No
	AN48						Yes No
	AO48						Yes No
	AP48						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	48	Brown, Robert D. and Martin, Yvonne C., "Designing Combinatorial Library Mixtures Using a Genetic Algorithm," *J. Med. Chem.*, 1997, Vol. 40, pp. 2304-2313.
AM	AS	48	Brown, Robert D. and Martin, Yvonne C., "The Information Content of 2D and 3D Structural Descriptors Relevant to Ligand-Receptor Binding," *J. Chem. Info. Comput. Sci.*, 1997, Vol. 37, pp. 1-9.
AM	AT	48	Brown, Robert D. and Martin, Yvonne C., "Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection," *J. Chem. Inf. Sci.*, 1996, Vol. 36, pp. 572-584.

EXAMINER Andrew Massad DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA49						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL49						Yes No
	AM49						Yes No
	AN49						Yes No
	AO49						Yes No
	AP49						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	49	Cummins, David J. *et al.*, "Molecular Diversity in Chemical Databases: Comparison of Medicinal Chemistry Knowledge Bases and Databases of Commercially Available Compounds," *American Chemical Society*, 1996, 14 pages.
AM	AS	49	*Daylight Theory: Fingerprints* (visited September 26, 2000) <http://www.daylight.com/dayhtml/doc/theory/theory.finger.html>, 8 pages.
AM	AT	49	*Daylight Theory: SMARTS* (visited September 26, 2000) <http://www.daylight.com/dayhtml/doc/theory/theory.smarts.html>, 10 pages.

EXAMINER	Justin Marsden	DATE CONSIDERED	9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL50						Yes No
	AM50						Yes No
	AN50						Yes No
	AO50						Yes No
	AP50						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	50	Downs, Geoff M. and Barnard, John M., "Techniques for Generating Descriptive Fingerprints in Combinatorial Libraries," *J. Chem. Inf. Comput. Sci.*, 1997, Vol. 37, pp. 59-61.
AM	AS	50	Gillet, Valerie J., "Background Theory of Molecular Diversity," *Molecular Diversity in Drug Design*, 1999, pp. 43-65.
AM	AT	50	Good, Andrew C. and Lewis, Richard A., "New Methodology for Profiling Combinatorial Libraries and Screening Sets: Cleaning Up the Design Process with HARPick," *J. Med. Chem.*, 1997, Vol. 40, pp. 3926-3936.

EXAMINER Andi Mansley — DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL51						Yes No
	AM51						Yes No
	AN51						Yes No
	AO51						Yes No
	AP51						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	51	Gorse, Dominique and Lahana, Roger, "Functional diversity of compound libraries," *Current opinion in chemical biology*, 2000, Vol. 4, pp. 287-294.
AM	AS	51	Jamois, Eric A. *et al.*, "Evaluation of Reagent-Based and Product-Based Strategies in the Design of Combinatorial Library Subsets," *J. Chem. Inf. Comput. Sci.*, December 9, 1999, Vol. 40, pp. 63-70.
AM	AT	51	Leach, Andrew R. *et al.*, "Implementation of a System for Reagent Selection and Library Enumeration, Profiling, and Design," *J. Chem. Inf. Comput. Sci.*, October 29, 1999, Vol. 39, pp. 1161-1172.

EXAMINER	Andi Maasley	DATE CONSIDERED	9/23/02

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	APPLICANT Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA52						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL52						Yes No
	AM52						Yes No
	AN52						Yes No
	AO52						Yes No
	AP52						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	52	Leach, Andrew R. and Hann, Michael M., "The *in silico* world of virtual libraries," *Drug discovery today*, August 2000, Vol. 5, pp. 326-336.
AM	AS	52	Leland, Burton A. *et al.*, "Managing the Combinatorial Explosion," *J. Chem. Inf. Comput. Sci.*, 1997, Vol. 37, pp. 62-70.
AM	AT	52	Lobanov, Victor S. and Agrafiotis, Dimitris K., "Stochastic Similarity Selections from Large Combinatorial Libraries," *J. Chem. Inf. Comput. Sci.*, January 21, 2000, Vol. 40, pp. 460-470.

EXAMINER	Andrei Marasoiu	DATE CONSIDERED	9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA53						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL53						Yes No
	AM53						Yes No
	AN53						Yes No
	AO53						Yes No
	AP53						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	53	Matter, Hans and Pötter, Thorsten, "Comparing 3D Pharmacophore Triplets and 2D Fingerprints for Selecting Diverse Compound Subsets," *J. Chem. Inf. Comput. Sci.*, October 29, 1999, Vol. 39, pp. 1211-1225.
AM	AS	53	Matter, Hans, "Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-Dimensional and Three-Dimensional Molecular Descriptors," *J. Med. Chem.*, 1997, Vol. 40, pp. 1219-1229.
AM	AT	53	Sadowski, Jens and Kubinyi, Hugo, "A Scoring Scheme for Discriminating between Drugs and Nondrugs," *J. Med. Chem.*, August 1, 1998, Vol. 41, pp. 3325-3329.

EXAMINER Andrew Marshall	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
	FILING DATE February 18, 2000	GROUP 1631

U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA54						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL54						Yes No
	AM54						Yes No
	AN54						Yes No
	AO54						Yes No
	AP54						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	54	Schnur, Dora, "Design and Diversity Analysis of Large Combinatorial Libraries Using Cell-Based Methods," *J. Chem. Inf. Comput. Sci.*, January 6, 1999, Vol. 39, pp. 36-45.
AM	AS	54	Schuffenhauer, Ansgar *et al.*, "Similarity Searching in Files of Three-Dimensional Chemical Structures: Analysis of the BIOSTER Database Using Two-Dimensional Fingerprints and Molecular Field Descriptors," *J. Chem. Inf. Comput. Sci.*, December 22, 1999, Vol. 40, pp. 295-307.
AM	AT	54	Turner, David B. *et al.*, "Rapid Quantification of Molecular Diversity for Selective Database Acquisition," *J. Chem. Inf. Sci.*, 1997, Vol. 37, pp. 18-22.

EXAMINER Andrew Marasley	DATE CONSIDERED 9/23/02

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FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL55						Yes No
	AM55						Yes No
	AN55						Yes No
	AO55						Yes No
	AP55						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	55	Wang, Jing and Ramnarayan, Kal, "Toward Designing Drug-Like Libraries: A Novel Computational Approach for Prediction of Drug Feasibility of Compounds," *J. Comb. Chem.*, October 19, 1999, Vol. 1, pp. 524-533.
AM	AS	55	Gasteiger *et al*, "Assessment of the Diversity of Combinatorial Libraries by an Encoding of Molecular Surface Properties," *Abstracts of Papers, American Chemical Society*, 211th ACS National Meeting, Item 070, March 1996.
AM	AT	55	Hassan, Moises *et al.*, "Optimization and visualization of molecular diversity of combinatorial libraries," *Molecular Diversity*, 1996, Vol. 2, pp. 64-74.

EXAMINER	Andrew Mansoor	DATE CONSIDERED	9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449 INFORMATION DISCLOSURE STATEMENT	ATTY. DOCKET NO. 1503.0730000	APPLICATION NO. 09/506,741
	APPLICANT Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA56						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL56						Yes No
	AM56						Yes No
	AN56						Yes No
	AO56						Yes No
	AP56						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	56	de Ridder, D. and Duin, R.P.W., "Sammon's mapping using neural networks: A comparison," *Pattern Recognition Letters*, Vol. 18, No. 11-13, 1997, pp. 1307-1316.
AM	AS	56	Kim, H. *et al.*, "Self-Organized Distributed Networks for Learning Highly Nonlinear Mapping," *Intelligent Engineering Systems Through Artificial Neural Networks*, Vol. 4, November 13-16, 1994, pp. 109-114.
AM	AT	56	Pal, N.R. and Eluri, V.K., "Two Efficient Connectionist Schemes for Structure Preserving Dimensionality Reduction," *IEEE Transactions on Neural Networks*, Vol. 9, No. 6, November 1998, pp. 1142-1154.

EXAMINER Andrew Mansfield	DATE CONSIDERED 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

FORM PTO-1449

INFORMATION DISCLOSURE STATEMENT

ATTY. DOCKET NO.	APPLICATION NO.
1503.0730000	09/506,741
APPLICANT: Lobanov *et al.*	
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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
AM	AA57	6,185,506 B1	02/2001	Cramer *et al.*	702	19	
	AB57						
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	AJ57						
	AK57						

FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL57						Yes No
	AM57						Yes No
	AN57						Yes No
	AO57						Yes No
	AP57						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

AM	AR	57	Clark, R., *et al.*, "Visualizing Substructural Fingerprints," *Journal of Molecular Graphics and Modelling*, Vol. 18, Elsevier Science, Inc., New York, New York, August-October, 2000, pp. 404-411.
AM	AS	57	Domine, D. *et al.*, "Non-Linear Mapping for Structure-Activity and Structure-Property Modelling," *Journal of Chemometrics*, Vol. 7, No. 4, John Wiley & Sons, Ltd., July-August 1993, pp. 227-242.
AM	AT	57	Lobanov, V.S. and Agrafiotis, D.K., "Stochastic Similarity Selections from Large Combinatorial Libraries," *J. Chem. Inf. Comput. Sci.*, Vol. 40, No. 2, American Chemical Society, 2000 (published on Web January 21, 2000), pp. 460-470.

EXAMINER: Sadhna Marachy — DATE CONSIDERED: 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

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FORM PTO-1449

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U.S. PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUB-CLASS	FILING DATE
	AA58						
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FOREIGN PATENT DOCUMENTS

EXAMINER INITIAL		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUB-CLASS	TRANSLATION
	AL58						Yes No
	AM58						Yes No
	AN58						Yes No
	AO58						Yes No
	AP58						Yes No

OTHER (Including Author, Title, Date, Pertinent Pages, etc.)

	~~AR~~	~~58~~	~~Copy of International Search Report issued February 9, 2001 for PCT/US 00/07306, 5 pages.~~
	AS	58	
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EXAMINER: Ardin Marschel

DATE CONSIDERED: 9/23/02

EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.